A New Framework to Quantify the Uncertainty in Inverse Problems

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Observational data

$$y_i = (Fu)(x_i) + e_i$$

where e_i is random variable. It's to recover u from y.

For industrial consideration:

- Data based observation: point-wise or patch measurement.
- Uncertain measurements: some amount of noisy data.

Take $F = I$ for example: imaging, denoising, surface fitting.

F to be forward operator, it's inverse problem.

Image processing

$$y_i = u(x_i) + e_i$$

- Wavelets, Rudin-Osher-Fatemi (ROF) model
- Compressed sensing(sparse method), e.g. Terence Tao
- Neural Networks

The observational data

The observational data: $y_i = u_0(x_i) + e_i,\ 1 \le i \le n$. u_0 comes from partial differential equations.

Given:

- noise e_i
- Large n, e.g. $n = 10^6$

Question:

- Recover u_0
- Error estimate

Applications: Data mining, interpolation, surface fitting, ...

Thin plate spline model

Data $y_i = u_0(x_i) + e_i,\ 1 \le i \le n$, Ω bounded domain of $\mathbf{R}^d$, $d \le 3$.

D^2-spline:

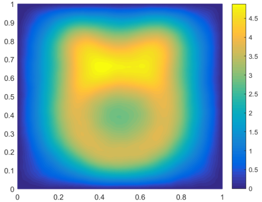
$$\min_{u \in H^2(\Omega)} \frac{1}{n} \sum_{i=1}^{n} (u(x_i) - y_i)^2 + \lambda_n |u|^2_{H^2(\Omega)},$$

where $\lambda_n > 0$.

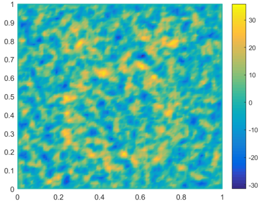
- The choice of λ_n
- Discrete method
- Error estimate

The choice of λ_n

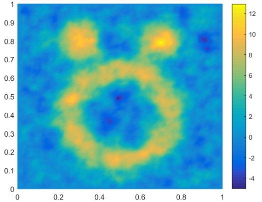
Take inverse parabolic source problem for example:



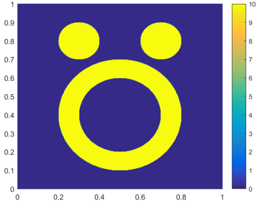
(a) $\lambda_n = 10^{-4}$ too big, over smooth



(b) $\lambda_n = 10^{-7}$ too small, over fit



(c) $\lambda_n = 1.5 \times 10^{-6}$



(d) true image

Error estimate

If $\{e_i\}_{i=1}^n$ s.t. $\mathbb{E}[e_i] = 0$ and $\mathbb{E}[e_i^2] \leq \sigma^2$. Define $\|u\|_n^2 = \frac{1}{n}\sum_{i=1}^n u^2(x_i)$.

Theorem

Let $u_n \in H^2(\Omega)$ be the unique solution of the thin plate spline model. Then there exist constants $\lambda_0 > 0$ and $C > 0$ s.t. for any $\lambda_n \leq \lambda_0$ and $n\lambda_n^{d/4} \geq 1$,

$$\mathbb{E}\left[\|u_n - u_0\|_n^2\right] \leq C\lambda_n |u_0|_{H^2(\Omega)}^2 + \frac{C\sigma^2}{n\lambda_n^{d/4}},$$

Optimal smoothing parameter:

$$\lambda_n^{1+d/4} = O((\sigma^2 n^{-1})|u_0|_{H^2(\Omega)}^{-2}).$$

Finite element for spline model

e.g. $u_0 = (xy)^{1.501} \in H^2((0,1)\times(0,1))$, $n = 10^6$, $\sigma = 0.1$.

$$\lambda_n^{1+d/4} = O((\sigma^2 n^{-1})|u_0|_{H^2(\Omega)}^{-2}).$$

Optimal $\lambda_n \approx 2 \times 10^{-6}$,
Mesh size $h = O(\lambda_n^{1/4}) \approx 0.04$

$$Ax = y$$

- Radial basis: A, $10^6 \times 10^6$, full matrix
- **Finite element method:** A, 3000×3000, sparse matrix

Numerical examples

Optimal λ_n:

$$\lambda_n^{1/2+d/8} = O(\sigma n^{-1/2}(|u_0|_{H^2(\Omega)})^{-1}),$$

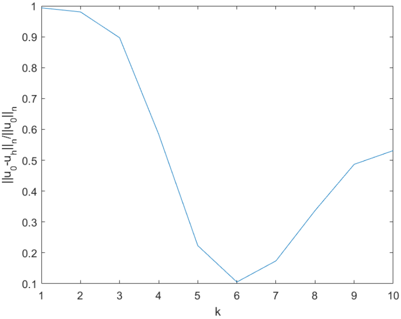


Figure: $u_0 = \sin(2\pi x^2 + 3\pi y)e^{x^3+y}$. *The relative error* $\|u_h - u_0\|_n / \|u_0\|_n$ *for different* $\lambda_n = 10^{-k}$. $\sigma n^{-1/2} = 1/50$. $\lambda_n^{opt} \approx 2.4 \times 10^{-6}$.

The smoothing parameter λ_n

$$\lambda_n^{1/2+d/8} = O(\sigma n^{-1/2}(|u_0|_{H^2(\Omega)})^{-1}).$$

- σ, u_0 unknow
- How to determine λ_n

Algorithm

(Self-consistent algorithm for finding λ_n)

1° *Initial guess* $\lambda_{n,0}$;

2° *For* $k \geq 0$ *and* $\lambda_{n,k}$, *compute* u_h *with* $\lambda_{n,k}$ *and* $h = \lambda_{n,k}^{1/4}$;

3° *Update* $\lambda_{n,k+1}^{1/2+d/8} = \|u_h - y\|_n n^{-1/2}(|u_h|_{2,h})^{-1}$.

The smoothing parameter λ_n

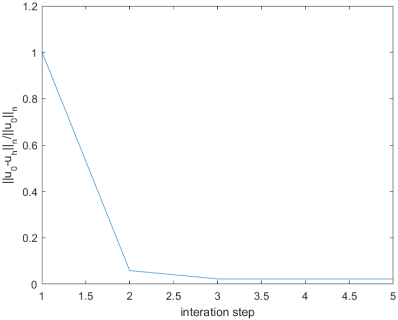


Figure: $u_0 = \sin(2\pi x^2 + 3\pi y)e^{x^3+y}$, $n = 10^6$, $\sigma = 1$. $\lambda_{n,5} = 4.3496e - 08$, *the optimal* $\lambda_n = 4.5054e - 08$

General model

$$m_i = (Sf^*)(x_i) + e_i, \;\; i = 1, 2, \cdots, n,$$

where $e = (e_1, e_2, \cdots, e_n)^T$ is the data noise vector, with $\{e_i\}_{i=1}^n$ being independent random variables. S is the forward operator from X to Y.

We look for an approximate solution f_n of the unknown source function f^* through the least-squares regularized minimization:

$$\min_{f \in X} \frac{1}{n} \sum_{i=1}^{n} |(Sf)(x_i) - m_i|^2 + \lambda_n \|f\|_X^2,$$

where $\lambda_n > 0$ is called a regularization parameter.

General model

Assumption

We assume that

(1) There exists a constant $\beta > 1$ such that for all $u \in Y$,

$$\|u\|^2_{L^2(\Omega)} \le C(\|u\|^2_n + n^{-\beta}\|u\|^2_Y), \quad \|u\|^2_n \le C(\|u\|^2_{L^2(\Omega)} + n^{-\beta}\|u\|^2_Y). \quad (1)$$

(2) The first n eigenvalues, $0 < \eta_1 \le \eta_2 \le \cdots \le \eta_n$, of the eigenvalue problem

$$(\psi, v)_X = \eta\,(S\psi, Sv) \ \ \forall v \in X,$$

satisfy that $\eta_k \ge Ck^\alpha$ $(k = 1, 2, \cdots, n)$ for some constant C depending only on the operator $S : X \to Y$ and the index α such that $1 < \alpha \le \beta$.

General model

Theorem

Let $f_n \in X$ be the unique solution of the inverse problem. Then there exist constants $\lambda_0 > 0$ and $C > 0$ such that for any $\lambda_n \leq \lambda_0$,

$$\mathbb{E}\left[\|Sf_n - Sf^*\|_n^2\right] \leq C\lambda_n \|f^*\|_X^2 + C\sigma^2/(n\lambda_n^{1/\alpha}),$$

$$\mathbb{E}\left[\|f_n\|_X^2\right] \leq C\|f^*\|_X^2 + C\sigma^2/(n\lambda_n^{1+1/\alpha}).$$

General model

Assumption

For a unit ball SY in Y and any $\varepsilon > 0$, there exists a constant $\gamma < 2$ such that the covering entropy is controlled by

$$\log N(\varepsilon, SY, \|\cdot\|_{L^\infty(\Omega)}) \leq C\varepsilon^{-\gamma}.$$

General model

Theorem

Let $\rho_0 = \|f^*\|_X + \sigma n^{-1/2}$*, and* $f_n \in X$ *be the solution of the minimization problem. If we take* $\lambda_n^{1/2+\gamma/4} = O(\sigma n^{-1/2} \rho_0^{-1})$*, then there exists a constant* $C > 0$ *such that*

$$\mathbb{P}(\|Sf_n - Sf^*\|_n \geq \lambda_n^{1/2} \rho_0 z) \leq 2\, e^{-Cz^2} \text{ and } \mathbb{P}(\|f_n\|_X \geq \rho_0 z) \leq 2\, e^{-Cz^2}.$$

General model

We can directly verify that the solution $f_n \in X$ satisfies the weak formulation

$$\lambda_n(f_n, v)_X + (Sf_n, Sv)_n = (m, Sv)_n \quad \forall v \in X\,.$$

Let $V_h \subset X$ and $Y_h \subset Y$ be two discrete function spaces (e.g., finite element spaces) with dimensions N_h and M_h.

$S_h : X \to Y_h \subset Y$ be the discrete approximation.

General model

Assumption

For the discrete operator $S_h : X \to Y_h \subset Y$,
(1) there exists an error estimate $e(h)$ *such that the discrete operator* S_h *satisfies*

$$\|Sf - S_h f\|_n^2 \le Ce(h)\|f\|_X^2 \;\forall f \in X\,.$$

(2) For any $f \in X$, *there exists* $v_h \in V_h$ *such that*

$$\lambda_n\|f - v_h\|_X^2 + \|S_h f - S_h v_h\|_n^2 \le C(\lambda_n + e(h))\|f\|_X^2.$$

General model

Theorem

$$
\begin{aligned}
\mathbb{E}\left[\|Sf^* - S_h f_h\|_n^2\right] &\leq C(\lambda_n + e(h))\|f^*\|_X^2 \\
&\quad + C\left[1 + \frac{e(h)}{\lambda_n} + \frac{N_h e(h)}{\lambda_n^{1-1/\alpha}}\right]\frac{\sigma^2}{n\lambda_n^{1/\alpha}}, \\
\mathbb{E}\left[\|f^* - f_h\|_X^2\right] &\leq C\frac{\lambda_n + e(h)}{\lambda_n}\|f^*\|_X^2 \\
&\quad + C\left[1 + \frac{e(h)}{\lambda_n} + \frac{N_h e(h)}{\lambda_n^{1-1/\alpha}}\right]\frac{\sigma^2}{n\lambda_n^{1+1/\alpha}}.
\end{aligned}
$$

In particular, if $e(h) \leq C\lambda_n$ *and* $N_h e(h) \leq C\lambda_n^{1-1/\alpha}$*, we have*

$$
\begin{aligned}
\mathbb{E}\left[\|Sf^* - S_h f_h\|_n^2\right] &\leq C\lambda_n\|f^*\|_X^2 + C\sigma^2/(n\lambda_n^{1/\alpha}), \\
\mathbb{E}\left[\|f^* - f_h\|_X^2\right] &\leq C\|f^*\|_X^2 + C\sigma^2/(n\lambda_n^{1+1/\alpha}).
\end{aligned}
$$

General model

Theorem

Let $f_h \in V_h$ be the solution of discrete problem. Denote by $\rho_0 = \|f^*\|_X + \sigma n^{-1/2}$. If we take $e(h) \le C\lambda_n$, $N_h e(h) \le C\lambda_n^{1-\gamma/2}$ and $\lambda_n^{1/2+\gamma/4} = O(\sigma n^{-1/2}\rho_0^{-1})$, then there exists a constant $C > 0$ such that for any $z > 0$,

$$\mathbb{P}(\|S_h f_h - Sf^*\|_n \ge \lambda_n^{1/2}\rho_0 z) \le 2e^{-Cz^2} \text{ and } \mathbb{P}(\|f_h\|_X \ge \rho_0 z) \le 2e^{-Cz^2}.$$

Inverse source problem in $\mathbb{R}^d$, $d \leq 3$

$$\begin{cases} u_t + Lu = f(x)g(t) \quad \text{in } \Omega \times (0, T), \\ u(x,t) = 0 \quad \text{on } \partial\Omega \times (0, T), \qquad u(x,0) = 0 \quad \text{in } \Omega, \end{cases}$$

Here $Lu = -\nabla \cdot (a(x)\nabla u) + c(x)u$ and $Sf = u(\cdot, T)$ is final time measurements.

The inverse problem is to recover the source $f(x)$ form the final time measurements:

$$y_i = Sf(x_i) + e_i$$

Inverse source problem

The least-squares regularized minimization:

$$\min_{f \in L^2(\Omega)} \frac{1}{n} \sum_{i=1}^{n} |(Sf)(x_i) - m_i|^2 + \lambda_n \|f\|_{L^2(\Omega)}^2,$$

1. Eigenvalue distributions of elliptic operators —— Expectation

$$L\psi = \mu\,\psi \;\text{ in } \Omega, \quad \psi = 0 \;\text{ on } \partial\Omega$$

   has a countable set of positive eigenvalues $C_1 k^{2/d} \leq \mu_k \leq C_2 k^{2/d}$.

2. Covering number of function space——Exponential decay tail

$$\log N(\varepsilon, SW^{2,2}(Q), \|\cdot\|_{L^\infty(Q)}) \leq C\varepsilon^{-1},$$

Inverse source problem

Theorem

For the minimizer $f_n \in L^2(\Omega)$, there exist constants $\lambda_0 > 0$ and $C > 0$ such that the following estimates hold for any $\lambda_n \leq \lambda_0$:

$$\begin{aligned} \mathbb{E}\left[\|Sf_n - Sf^*\|_n^2\right] &\leq C\lambda_n \|f^*\|^2_{L^2(\Omega)} + C\sigma^2/(n\lambda_n^{d/4}), \\ \mathbb{E}\left[\|f_n\|^2_{L^2(\Omega)}\right] &\leq C\|f^*\|^2_{L^2(\Omega)} + C\sigma^2/(n\lambda_n^{1+d/4}). \end{aligned}$$

Moreover, if $\lambda_n \geq n^{-4/d}$ and $g > 0$ in $[0, T]$, then

$$\mathbb{E}\left[\|f_n - f^*\|^2_{H^{-1}(\Omega)}\right] \leq C\lambda_n^{1/2} \|f^*\|^2_{L^2(\Omega)} + C\sigma^2/(n\lambda_n^{1/2+d/4}).$$

Inverse source problem

Theorem

Let $\rho_0 = \|f^*\|_{L^2(\Omega)} + \sigma n^{-1/2}$*. If we take* λ_n *such that* $\lambda_n^{1/2+d/8} = O(\sigma n^{-1/2}\rho_0^{-1})$*, then the following estimates hold for some constant* $C > 0$*:*

$$\mathbb{P}(\|Sf_n - Sf^*\|_n \geq \lambda_n^{1/2}\rho_0 z) \leq 2e^{-Cz^2}, \quad \mathbb{P}(\|f_n\|_{L^2(\Omega)} \geq \rho_0 z) \leq 2e^{-Cz^2}.$$

Moreover, if $\lambda_n \geq n^{-4/d}$ *and* $g > 0$ *in* $[0, T]$*, then*

$$\mathbb{P}(\|f_n - f^*\|_{H^{-1}(\Omega)} \geq \lambda_n^{1/4}\rho_0 z) \leq 2e^{-Cz^2}.$$

Finite element method

We use the backward Euler scheme

$$\Big(\frac{u_h^i - u_h^{i-1}}{\tau}, v_h\Big) + a(u_h^i, v_h) = (fg^i, v_h) \quad \forall v_h \in V_h,$$

where $a(v, w) = (a\nabla v, \nabla w) + (cv, w)$ for any $v, w \in H_0^1(\Omega)$.
The classical theory requires the regularity $\partial_{tt} u \in L^1(0, T; L^2(\Omega))$ of the solution of the problem, but this will not be guaranteed in this case. We show that

$$\|S_{\tau,h} f - Sf\|_{L^2(\Omega)} \leq C(h^2 + \tau|\ln\tau|)\|f\|_{L^2(\Omega)},$$

Finite element method

Theorem

Let $g \in H^2(0,T)$. $\{e_i\}_{i=1}^n$ are independent random variables satisfying $\mathbb{E}[e_i] = 0$ and $\mathbb{E}[e_i^2] \le \sigma^2$. Then there exist constants $\lambda_0 > 0$ and $C > 0$ such that for any $\lambda_n \le \lambda_0$ and $\tau|\ln\tau| = O(h^2)$, the following estimates hold:

$$\mathbb{E}\big[\|Sf^* - S_{\tau,h}f_h\|_n^2\big] \le C(\lambda_n + h^4)\|f^*\|_{L^2(\Omega)}^2 + C\left(1 + \frac{h^4}{\lambda_n}\right)\frac{\sigma^2}{n\lambda_n^{d/4}}.$$

Moreover, if $\lambda_n \ge n^{-4/d}$ and $g > 0$ in $[0,T]$, we have

$$\mathbb{E}\big[\|f^* - f_h\|_{H^{-1}(\Omega)}^2\big] \le C(\lambda_n^{1/2} + h^2)\Big(1 + \frac{h^4}{\lambda_n}\Big)\|f^*\|_{L^2(\Omega)}^2 + C(\lambda_n^{1/2} + h^2)\Big(1 + \frac{h^4}{\lambda_n}\Big)\frac{\sigma^2}{n\lambda_n^{1+d/4}}.$$

Optimal choice

Optimal parameter choice predicted by theory in $\mathbb{R}^2$:

$$\lambda_n^{3/4} = \sigma n^{-1/2} \|f^*\|_{L^2(\Omega)}^{-1}.$$

Algorithm (Computing an estimate of the regularization parameter λ_n)

1° *Given an initial guess of* $\lambda_{n,0}$*; for* $j = 0, 1, \cdots,$ *do the following*
2° *Solve regularization problem for* f_h *with* λ_n *replaced by* $\lambda_{n,j}$ *over the mesh* $\mathcal{M}_h$*;*
3° *Update* $\lambda_{n,j+1}$*:* $\quad \lambda_{n,j+1}^{1/2+d/8} = n^{-1/2} \|S_{\tau,h} f_h - m\|_n \, \|f_h\|_{L^2(\Omega)}^{-1}.$

Numerical examples

We will test on the following L^2 function with no more derivatives, since we do not assume any further source condition:

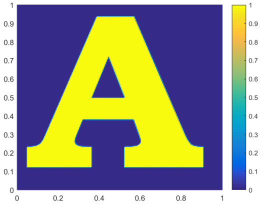


Figure: *The surface plot of the exact solution f^*.*

Numerical examples

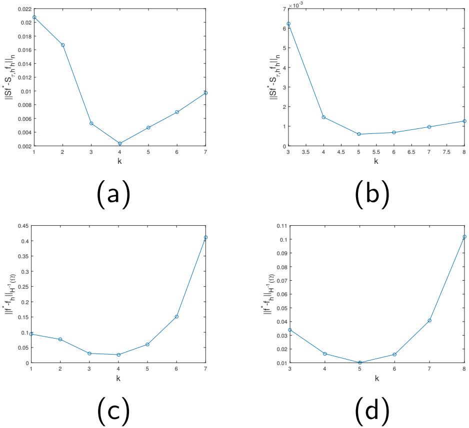
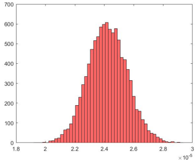
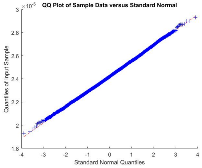


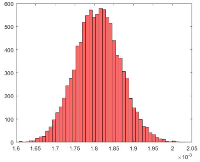
Figure: *Optimal choice are* $\lambda_n \approx 2.3 \times 10^{-4}$ *(for* $\sigma = 0.1$ *(a) and (c)) and* $\lambda_n \approx 1.1 \times 10^{-5}$ *(for* $\sigma = 0.01$ *(b) and (d)).*



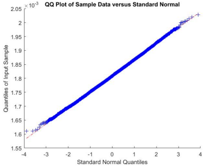
(a)



(b)



(c)



(d)

Figure: *(a) and (b) are the histogram (left) and quantile-quantile (right) plots of the empirical error* $\|S_{\tau,h}f_h - Sf^*\|_n$ *with* $10,000$ *samples. (c) and (d) are the histogram (left) and quantile-quantile (right) plots of the error* $\|f_h - f^*\|_{H^{-1}(\Omega)}$ *with* $10,000$ *samples.*

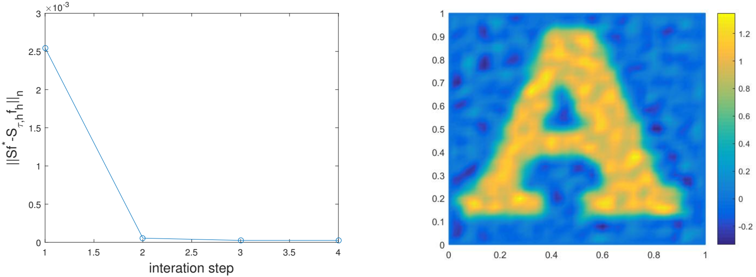
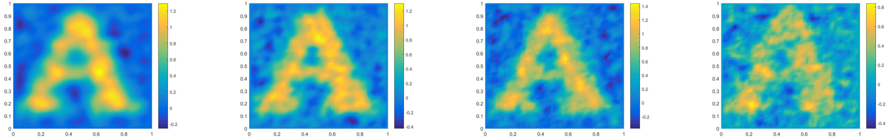


Figure: *The relative empirical error* $\|Sf^* - S_{\tau,h}f_h\|_n$ *at each iteration (left); The computed solution* f_h *at the end of iterations (right).*

Numerical examples



(a) (b) (c) (d)

Figure: *(a)-(d) are the computed solutions f_h when $T = 1,\ 0.1\ , 0.01,\ 0.001$, respectively.*

References

1. Z. Chen, R. Tuo and W. Zhang, Stochastic Convergence of A Nonconforming Finite Element Method for the Thin Plate Spline Smoother for Observational Data, SIAM Journal on Numerical Analysis, 2018, 56: 635-659.
2. Zhiming Chen, Wenlong Zhang, Jun Zou, Stochastic convergence of regularized solutions and their finite element approximations to inverse source problems, SIAM Journal on Numerical Analysis, 2022, 60(2), 751-780.

Thank you